

Identifying spin-triplet pairing in spin-orbit coupled multi-band superconductors

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Abstract – We investigate the combined effect of Hund’s and spin-orbit (SO) coupling on superconductivity in multi-orbital systems. Hund’s interaction leads to orbital-singlet spin-triplet superconductivity, where the Cooper pair wave function is antisymmetric under the exchange of two orbitals. We identify three *d*-vectors describing even-parity orbital-singlet spin-triplet pairings among t_{2g} -orbitals, and find that the three *d*-vectors are mutually orthogonal to each other. SO coupling further assists pair formation, pins the orientation of the *d*-vector triad, and induces spin-singlet pairings with a relative phase difference of $\pi/2$. In the band basis the pseudospin *d*-vectors are aligned along the *z*-axis and correspond to momentum-dependent inter- and intra-band pairings. We discuss quasiparticle dispersion, magnetic response, collective modes, and experimental consequences in light of the superconductor Sr_2RuO_4 .

Introduction. – Since its inception, standard Bardeen-Cooper-Schrieffer (BCS) theory has been considered a classic example for a collective phase emerging from quantum many body effects. However, the discovery of unconventional superconducting phases near antiferromagnetic order in heavy fermion compounds [1,2], organic materials [3], and, most recently, Fe-pnictides [4] have exposed the limits of a single-band BCS formulation. The origin and nature of superconductivity in complex materials where multiple bands cross the Fermi level therefore remains a field of active research, harbouring intriguing challenges and mysteries.

In particular, when the electronic structure near the Fermi energy is composed of different orbitals and spins mixed via spin-orbit (SO) coupling, a pairing symmetry analysis could be non-trivial. For example, a local microscopic interaction such as Hund’s coupling may naturally favour inter-orbital spin-triplet pairing between electrons. However, when orbital and spin fluctuations are significant due to inter-orbital hopping and SO interaction, pairing in definite orbital and spin channels (*e.g.*, spin-singlet or -triplet pairing between electron in orbitals *a* and *b*) is not well defined. Equivalently, from a Bloch band per-

spective, where the kinetic Hamiltonian including SO effects is diagonal, the decoupling of the microscopic interaction effectively leads to intra- and inter-band pairing with pseudospin-singlet and/or -triplet character.

Below we present a systematic study of how SO and Hund’s couplings jointly give rise to superconductivity in t_{2g} (*i.e.*, d_{yz} , d_{xz} , and d_{xy}) orbital systems. Our findings may apply to a number of multi-orbital *d*-subshell superconductors. To be specific we base our quantitative considerations on the proposed chiral spin-triplet superconductor Sr_2RuO_4 . Here, despite intense investigation for more than a decade, a clear picture for the pairing symmetry, the pairing mechanism and the relevant bands involved that is consistent with all experimental observations has not yet emerged [5,6].

The paper is organized as follows. In the second section we discuss Cooper pairing in multi-orbital systems. We find that superconductivity from local Hund’s exchange can naturally be characterized by three mutually orthogonal *d*-vectors each describing inter-orbital *even-parity spin-triplet* pairing. We then show how SO coupling pins the orientation of the *d*-vector triad and induces and enhances pairing via coupling to spin-singlet pairing order parameters with a fixed relative phase difference of $\pi/2$. In the third section, we map these local pairing order pa-

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rameters, defined in an orbital and spin basis, to inter- and intra-band pairing in the Bloch band basis. Pairing in the Bloch bands has a strong momentum dependence and the magnitude and direction of the d -vectors depend on the orbital composition at each \mathbf{k} -point. In the fourth section, we present the complete self-consistent mean-field (MF) results involving 9 complex order parameters using band structure parameters that reproduce the Fermi surface (FS) reported on Sr_2RuO_4 . In addition, the resulting anisotropic quasiparticle (QP) dispersion, the magnetic response and the critical pairing strengths in the presence of SO coupling are considered. We summarize our findings and discuss the relevance for SO-coupled d -orbital superconductors such as Sr_2RuO_4 in the last section.

Pairing in SO coupled t_{2g} systems via Hund's interaction. – For multi-orbital 3d-subshell systems such as the Fe-pnictides, it was recognized that Hund's coupling (interaction strength denoted by J) is as important as on-site Coulomb repulsion (U) [7, 8], while SO coupling (2λ) is relatively weak [9]. In contrast, recent x-ray measurements on 5d transition metal compounds such as Ir-based oxide materials found that the SO interaction of 0.6 eV is roughly comparable to the on-site Coulomb energy [10], suggesting that SO interaction is larger than Hund's exchange (since $J < U$). Given that the effective pairing interaction in the spin-triplet channel arising from Hund's coupling and inter-orbital Hubbard repulsion ($V = U - 2J$) scales as $V - J = U - 3J$ (see below), we therefore expect that for 4d-subshell materials such as Sr_2RuO_4 both SO and spin-triplet pairing interactions are intermediate in strength and of similar magnitude [11–17]. Since neither interaction is negligible nor dominant, we treat both on an equal footing in the present study.

While on-site Hund's and further neighbor exchange interactions have been recognized to be important for spin-triplet pairing [7, 18–21], the combined effect of SO and Hund's couplings on inter-orbital spin-triplet pairing has not been investigated in t_{2g} -orbital systems. To understand superconductivity in SO coupled t_{2g} -orbital systems, we consider a generic Hamiltonian $H = H_{\text{kin}} + H_{\text{SO}} + H_{\text{int}}$ consisting of kinetic, SO, and local Kanamori interaction terms. In this section we leave the kinetic Hamiltonian H_{kin} unspecified and focus on the pairing properties arising from the interplay of the atomic SO coupling $H_{\text{SO}} = 2\lambda \sum_i \mathbf{L}_i \cdot \mathbf{S}_i$ and the local interaction, which, projected on the t_{2g} orbitals, are given by

$$\begin{aligned} H_{\text{SO}} &= i\lambda \sum_i \sum_{abl} \epsilon_{abl} c_{i\sigma}^{a\dagger} c_{i\sigma'}^b \hat{\sigma}_{\sigma\sigma'}^l, \\ H_{\text{int}} &= \frac{U}{2} \sum_{i,a} c_{i\sigma}^{a\dagger} c_{i\sigma'}^{a\dagger} c_{i\sigma}^a c_{i\sigma'}^a + \frac{V}{2} \sum_{i,a \neq b} c_{i\sigma}^{a\dagger} c_{i\sigma'}^{b\dagger} c_{i\sigma}^b c_{i\sigma'}^a \\ &\quad + \frac{J}{2} \sum_{i,a \neq b} c_{i\sigma}^{a\dagger} c_{i\sigma'}^{b\dagger} c_{i\sigma}^a c_{i\sigma'}^b + \frac{J'}{2} \sum_{i,a \neq b} c_{i\sigma}^{a\dagger} c_{i\sigma'}^{a\dagger} c_{i\sigma}^b c_{i\sigma'}^b. \end{aligned} \quad (1)$$

Here and in the following, summation over repeated spin

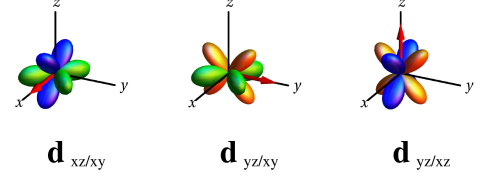


Fig. 1: (Color online) The orbital-singlet spin-triplet d -vectors form a triad whose orientation is pinned along $\hat{\mathbf{x}}$, $\hat{\mathbf{y}}$, and $\hat{\mathbf{z}}$ (or $-\hat{\mathbf{x}}$, $-\hat{\mathbf{y}}$, and $-\hat{\mathbf{z}}$) in the presence of SO coupling. See main text for details.

indices $\sigma, \sigma' = \uparrow, \downarrow$ is implied while the indices $a, b \in \{yz, xz, xy\}$ belong to an ordered set of t_{2g} -orbitals. Furthermore, $\hat{\sigma}^l$ stands for Pauli matrices, $c_{i\sigma}^{a\dagger}$ creates an electron on site i in orbital a with spin σ , and ϵ_{abl} denotes the totally antisymmetric rank-3 tensor. For transparency we have also introduced separate interaction strengths for Hund's coupling (J) and pair hopping (J'), although $J = J'$ at the atomic level.

Let us apply a MF approach to study the particle-particle instabilities of the microscopic interaction H_{int} using the following zero momentum pairing channels

$$\hat{\Delta}_{a/b}^s = \frac{1}{4N} \sum_{\mathbf{k}} [i\hat{\sigma}^y]_{\sigma\sigma'} (c_{\mathbf{k}\sigma}^a c_{-\mathbf{k}\sigma'}^b + c_{\mathbf{k}\sigma}^b c_{-\mathbf{k}\sigma'}^a), \quad (3)$$

$$\hat{d}_{a/b}^l = \frac{1}{4N} \sum_{\mathbf{k}} [i\hat{\sigma}^y \hat{\sigma}^l]_{\sigma\sigma'} (c_{\mathbf{k}\sigma}^a c_{-\mathbf{k}\sigma'}^b - c_{\mathbf{k}\sigma}^b c_{-\mathbf{k}\sigma'}^a), \quad (4)$$

where N is the number of \mathbf{k} points. Here, $\Delta_{a/b}^s = \langle \hat{\Delta}_{a/b}^s \rangle$ ($= \Delta_{b/a}^s$) stands for intra- ($a = b$) and inter-orbital ($a \neq b$) spin-singlet pairing, which is even under the exchange of orbital quantum numbers (*i.e.* they form “orbital triplets”). The vector order parameter $\mathbf{d}_{a/b} = (\langle \hat{d}_{a/b}^x \rangle, \langle \hat{d}_{a/b}^y \rangle, \langle \hat{d}_{a/b}^z \rangle)$ ($= -\mathbf{d}_{b/a}$) on the other hand parametrizes inter-orbital ($a \neq b$) spin-triplet pairing consistent with the usual d -vector notation where $i(\mathbf{d} \cdot \hat{\sigma})\hat{\sigma}^y$ describes the spin-triplet pairing gap [2, 22]. Note that $\mathbf{d}_{a/b}$ is odd under orbital exchange, which is characteristic of an “orbital singlet” (while $\mathbf{d}_{a/a} = 0$). Note also that the above order parameters are all even under a parity transformation as they are locally defined; this feature differs in particular from conventional odd-parity spin-triplet pairing where orbital degrees of freedom are absent.

Using the above pairing channels the interaction Hamiltonian takes the form

$$\begin{aligned} H_{\text{int}} \rightarrow & UN \sum_a \hat{\Delta}_{a/a}^{s\dagger} \hat{\Delta}_{a/a}^s + (V - J)N \sum_{a,b,l} \hat{d}_{a/b}^{l\dagger} \hat{d}_{a/b}^l \\ & + J'N \sum_{a \neq b} \hat{\Delta}_{a/a}^{s\dagger} \hat{\Delta}_{b/b}^s + (V + J)N \sum_{a \neq b} \hat{\Delta}_{a/b}^{s\dagger} \hat{\Delta}_{a/b}^s, \end{aligned} \quad (5)$$

where it is clear that only Hund's coupling can give rise to an instability in a spin-triplet channel [7, 19]. We thus

concentrate on the effective pairing interaction

$$H'_{\text{int}} = (U - 3J)N \sum_{a,b,l} \hat{d}_{a/b}^\dagger \hat{d}_{a/b}^l \quad (6)$$

in the attractive regime $U/3 < J (< U)$. In general, orbital-singlet spin-triplet pairing can also induce spin-singlet pairing so that the remaining terms in Eq. (5) would hamper spin-singlet pairing. However, we assume that their effect is negligible to keep the following self-consistent calculations feasible, and since the induced spin-singlet pairing amplitudes are for the most part smaller than the spin-triplet pairing amplitudes (see below). For notational clarity we label in the following inter-orbital pairing only by the three combinations $a/b = xz/xy, yz/xy, yz/xz$.

To understand the effect of SO interaction, let us remark on pairing in the absence of SO coupling first. In the case of the layered compound considered below (and for a rather large parameter range) the three spin-triplet d -vectors $\mathbf{d}_{xz/xy}$, $\mathbf{d}_{yz/xy}$, and $\mathbf{d}_{yz/xz}$ form a triad of mutually orthogonal vectors with an arbitrary orientation and chirality in spin space, and no relative complex phase difference (hence preserving time reversal symmetry (TRS)). This can be understood by analyzing the Ginzburg-Landau (GL) free energy, which without SO coupling is given by

$$\begin{aligned} \mathcal{F} \sim & \sum_{\nu} [A_{\nu} |\mathbf{d}_{\nu}|^2 + B_{\nu}^{(1)} (\mathbf{d}_{\nu} \cdot \mathbf{d}_{\nu}^*)^2 + B_{\nu}^{(2)} |\mathbf{d}_{\nu} \cdot \mathbf{d}_{\nu}|^2] \\ & + \sum_{\nu \neq \kappa} [C_{\nu\kappa}^{(1)} (\mathbf{d}_{\nu} \cdot \mathbf{d}_{\nu})(\mathbf{d}_{\kappa} \cdot \mathbf{d}_{\kappa})^* + C_{\nu\kappa}^{(2)} |\mathbf{d}_{\nu}|^2 |\mathbf{d}_{\kappa}|^2] \\ & + C_{\nu\kappa}^{(3)} |\mathbf{d}_{\nu} \cdot \mathbf{d}_{\kappa}|^2 + C_{\nu\kappa}^{(4)} |\mathbf{d}_{\nu} \cdot \mathbf{d}_{\kappa}^*|^2 + C_{\nu\kappa}^{(5)} (\mathbf{d}_{\nu} \cdot \mathbf{d}_{\kappa}^*)^2 \end{aligned} \quad (7)$$

up to fourth order, by analogy to He-3 [23]. Here ν, κ stand for orbital pairs a/b , while the (real) quartic mixing parameters obey $C_{\nu\kappa}^{(i)} = C_{\kappa\nu}^{(i)}$ and the asymmetry between in-plane and out-of-plane orbitals due to *e.g.* inter-orbital hopping is reflected in distinct coefficients ($A_{yz/xz} \neq A_{yz/xy} = A_{xz/xy}$, etc.). This form is dictated by gauge symmetry, SU(2) spin rotational symmetry, time reversal symmetry and the underlying lattice symmetries, and shows that the $C_{\nu\kappa}^{(3)}$ and $C_{\nu\kappa}^{(4)}$ terms are sensitive to the relative orientation of the d -vectors, whereas the $C_{\nu\kappa}^{(1)}$ and $C_{\nu\kappa}^{(5)}$ contributions additionally depend on their relative complex phases.

However, once SO coupling is included, $\mathbf{d}_{xz/xy}$, $\mathbf{d}_{yz/xy}$, and $\mathbf{d}_{yz/xz}$ are pinned along x , y , and z directions, respectively, as shown in fig. 1. Inversion/time reversal symmetry on the other hand is still preserved and reflected in the degeneracy of the orientations/chiralities $\{\mathbf{d}_{xz/xy}, \mathbf{d}_{yz/xy}, \mathbf{d}_{yz/xz}\}$ and $\{-\mathbf{d}_{xz/xy}, -\mathbf{d}_{yz/xy}, -\mathbf{d}_{yz/xz}\}$. The pinning of the d -vectors occurs due to additional terms in the free energy such as $\sim a^{(1)} |d_{yz/xz}^z|^2 + a^{(2)} [|d_{yz/xy}^z|^2 + |d_{xz/xy}^z|^2] + b^{(1)} [|d_{yz/xz}^x|^2 + |d_{yz/xz}^y|^2] + b^{(2)} [|d_{xz/xy}^x|^2 + |d_{yz/xy}^y|^2] +$

$c^{(1)} [d_{yz/xy}^x (d_{xz/xy}^y)^* + d_{yz/xy}^y (d_{xz/xy}^x)^* + \text{c.c.}] + \dots$, where the expansion parameters depend on the SO coupling strength, naively suggesting that $a^{(1)}, a^{(2)} < b^{(1)}, b^{(2)}, c^{(1)}$, etc.¹ SO interaction furthermore leads to a linear coupling between a particular component of (inter-orbital) spin-triplet pairing and (intra-orbital) spin-singlet pairing. For example, writing SO coupling between yz and xz orbitals in the form of $-i\lambda [\hat{\sigma}^z]_{\sigma\sigma'} (c_{\mathbf{k}\sigma}^{yz\dagger} c_{\mathbf{k}\sigma'}^{xz} - c_{\mathbf{k}\sigma}^{xz\dagger} c_{\mathbf{k}\sigma'}^{yz})$ the following linear coupling is allowed in the GL free energy:

$$-i \lambda [\hat{\sigma}^z]_{\sigma\sigma'} \langle c_{\mathbf{k}\sigma}^{yz\dagger} c_{\mathbf{k}\sigma'}^{xz} - c_{\mathbf{k}\sigma}^{xz\dagger} c_{\mathbf{k}\sigma'}^{yz} \rangle \quad (8)$$

$$\times [i\hat{\sigma}^y \hat{\sigma}^z]_{\sigma\sigma'} \langle c_{\mathbf{k}\sigma}^{yz} c_{-\mathbf{k}\sigma'}^{xz} - c_{\mathbf{k}\sigma}^{xz} c_{-\mathbf{k}\sigma'}^{yz} \rangle$$

$$\times \left([i\hat{\sigma}^y]_{\sigma\sigma'} \langle c_{\mathbf{k}\sigma}^{yz\dagger} c_{-\mathbf{k}\sigma'}^{yz\dagger} \rangle + [i\hat{\sigma}^y]_{\sigma\sigma'} \langle c_{\mathbf{k}\sigma}^{xz\dagger} c_{-\mathbf{k}\sigma'}^{xz\dagger} \rangle \right)$$

$$\rightarrow i\lambda d_{yz/xz}^z \left(\Delta_{yz/yz}^s + \Delta_{xz/xz}^s \right)^* + \text{c.c.} \quad (9)$$

Note that $\mathbf{d}_{yz/xz}$ prefers the z -direction by coupling to spin-singlet pairing with a relative phase difference of $\pm\pi/2$ depending on the sign of λ . This is consistent with our findings below that the spin-triplet order parameters are purely real while the spin-singlet amplitudes are purely imaginary. A similar analysis can be carried out for $d_{xz/xy}^x$ and $d_{yz/xy}^y$. The overall order parameter for yz and xz orbitals then is $d_{xz/yz}^z + i(\Delta_{xz/xz}^s + \Delta_{yz/yz}^s)$. Since the relative phase between the orbital-triplet spin-singlet and the orbital-singlet spin-triplet order parameters is fixed, there should be a collective mode representing a resonance of supercurrent flow between the coupled order parameters with an energy scale of order $\sim \sqrt{|d_{a/b}^z|^2 + |\Delta_{a/a}^s|^2 + |\Delta_{b/b}^s|^2}$.

Note that the above result is fundamentally different from similar two orbital models, which lead to a single orbital-singlet spin-triplet d -vector [19,21,24]. The present model is also distinguished from other models where the momentum dependence in the band pairing usually originates from nonlocal momentum dependent interactions [18], whereas here it arises from spin and orbital mixing in the Bloch bands as described next.

Momentum-dependent pairing in the Bloch bands. — Despite having uniform pairing amplitudes $\mathbf{d}_{yz/xz}, \mathbf{d}_{yz/xy}, \mathbf{d}_{xz/xy}, \Delta_{yz/yz}^s, \dots$ the corresponding inter- and intra-band pairings in the Bloch band basis (now carrying band and pseudospin quantum numbers $-\eta, \rho = \alpha, \beta, \gamma$ and $s = \pm$) acquire a strong momentum dependence due to the mixing of orbitals through hopping and SO coupling. To understand how the above local pairing in the orbital and spin basis corresponds to pairing in the Bloch band basis, let us introduce the kinetic Hamiltonian. The most generic kinetic Hamiltonian for t_{2g} orbitals in a

¹Analyzing the energetics of a corresponding two orbital model one can indeed show that SO interaction tends to stabilize *e.g.* the $d_{yz/xz}^z$ -component over $d_{yz/xz}^x$ or $d_{yz/xz}^y$.

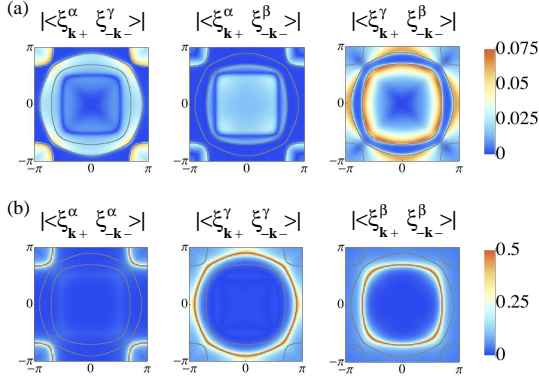


Fig. 2: (Color online) Momentum-resolved pairing amplitudes in the Bloch band basis for $3J - U = 0.9$ and $\lambda = 0.15$. Panel (a) and (b) represent inter- and intra-band pairing, respectively. The grey lines indicate the β , γ , and α FS sheets (from inside to outside). Note that pairing from Hund's coupling preferentially involves electronic states near the FS sheets and that the intra-band pairing amplitudes are about one order of magnitude larger than inter-band pairing amplitudes.

single layer perovskite structure has the form

$$H_{\text{kin}} + H_{\text{SO}} = \sum_{\mathbf{k}, \sigma} C_{\mathbf{k}\sigma}^\dagger \begin{pmatrix} \varepsilon_{\mathbf{k}}^{yz} & \varepsilon_{\mathbf{k}}^{1d} + i\lambda & -\lambda \\ \varepsilon_{\mathbf{k}}^{1d} - i\lambda & \varepsilon_{\mathbf{k}}^{xz} & i\lambda \\ -\lambda & -i\lambda & \varepsilon_{\mathbf{k}}^{xy} \end{pmatrix} C_{\mathbf{k}}(10)$$

where $C_{\mathbf{k}\sigma}^\dagger = (c_{\mathbf{k}\sigma}^{yz\dagger}, c_{\mathbf{k}\sigma}^{xz\dagger}, c_{\mathbf{k}\sigma}^{xy\dagger})$ and the dispersions are $\varepsilon_{\mathbf{k}}^{yz/xz} = -2t_1 \cos k_y/x - 2t_2 \cos k_x/y - \mu_1$, $\varepsilon_{\mathbf{k}}^{xy} = -2t_3 (\cos k_x + \cos k_y) - 4t_4 \cos k_x \cos k_y - \mu_2$, and $\varepsilon_{\mathbf{k}}^{1d} = -4t_5 \sin k_x \sin k_y$. For the MF calculation below we have chosen the parameters $t_1 = 0.5$, $t_2 = 0.05$, $t_3 = 0.5$, $t_4 = 0.2$, $t_5 = 0.05$, $\mu_1 = 0.55$, and $\mu_2 = 0.65$ (all energies here and in the following are expressed in units of $2t_1 = 1.0$). The underlying FS obtained from diagonalizing H_{kin} with SO coupling strength $\lambda = 0.15$ is shown in fig. 2 along with momentum-dependent band pairing amplitudes. The FS agrees well with first principles calculations [14] and the experimentally measured FS of Sr_2RuO_4 [17, 25, 26], consisting of three bands labelled α , β , and γ .

In the presence of SO coupling the bands are mixtures of all three orbitals and different spins, *e.g.* $\xi_{\mathbf{k}+}^\eta = \tilde{f}_{\mathbf{k}}^\eta c_{\mathbf{k}\uparrow}^{xz} + \tilde{g}_{\mathbf{k}}^\eta c_{\mathbf{k}\uparrow}^{yz} + \tilde{h}_{\mathbf{k}}^\eta c_{\mathbf{k}\downarrow}^{xy}$ ($\eta = \alpha, \beta, \gamma$). Hence considering inter- and intra-band pairing amplitudes in the band basis, it is clear that the x - and y -components of the inter-band pseudospin-triplets such as $\langle \xi_{\mathbf{k}+}^\eta \xi_{\mathbf{k}-}^\rho \rangle$ vanish, since $\langle d_{\mathbf{k}\uparrow}^{xz} d_{\mathbf{k}\uparrow}^{yz} \rangle$, $\langle d_{\mathbf{k}\uparrow}^{xz} d_{\mathbf{k}\downarrow}^{xy} \rangle$, and $\langle d_{\mathbf{k}\uparrow}^{yz} d_{\mathbf{k}\downarrow}^{xy} \rangle$ amplitudes are zero (similarly for $\uparrow \leftrightarrow \downarrow$). Thus only finite z -components of the three inter-band pseudospin-triplet d -vectors and inter-band pseudospin-singlet order parameters (such as $\langle \xi_{\mathbf{k}+}^\eta \xi_{\mathbf{k}-}^\rho \pm \xi_{\mathbf{k}+}^\rho \xi_{\mathbf{k}-}^\eta \rangle$) can appear. Figure 2 reveals that intra-band pairing is strongest and sharply peaked around the FS due to the mixing of all orbitals via SO interaction and inter-orbital hopping, and the ideal conditions for zero-momentum pairing. Inter-band pairing in contrast is about an order of magnitude weaker and, in particular for

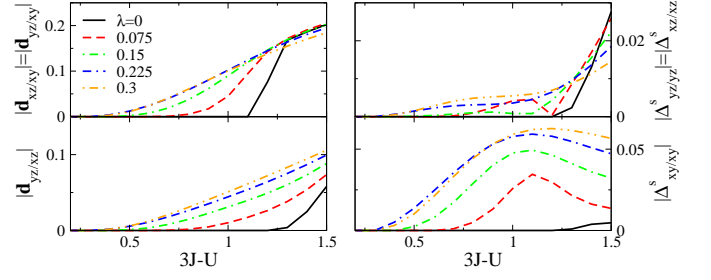


Fig. 3: (Color online) MF solutions for different SO coupling strengths for the Sr_2RuO_4 based band structure. Orbital-singlet spin-triplet pairing $\mathbf{d}_{xz/xy}$, $\mathbf{d}_{yz/xy}$, and $\mathbf{d}_{yz/xz}$ (purely real) induces finite intra-orbital spin-singlet pairing $\Delta_{yz/yz}^s$, $\Delta_{xz/xz}^s$, and $\Delta_{xy/xy}^s$ (purely imaginary). We also checked for induced inter-orbital spin-singlet pairing amplitudes, which, however, vanish.

$\langle \xi_{\mathbf{k}+}^\gamma \xi_{\mathbf{k}-}^\beta \rangle$, more spread out in momentum space, marking Bloch band states that are energetically still close enough to the FS to participate significantly in pairing.

This analysis demonstrates that inter-orbital pairing arising from Hund's interaction leads to \mathbf{k} -dependent inter- and intra-band pairing in pseudospin-singlet and pseudospin-triplet (z component only) channels. Furthermore, the pairing instability occurs simultaneously within and between all bands rather than in a single active band with superconductivity leaking into passive bands through, *e.g.*, pair hopping. The role of intra-band spin-triplet pairing between α and β bands in multi-orbital superconductors like Sr_2RuO_4 has also been the focus of recent studies, where the inter-band order parameter, however, breaks TRS [27] and an intrinsic anomalous Hall effect can contribute significantly to a large TRS breaking signal in Kerr rotation experiments [28, 29].

Pairing transition, QP dispersion, and magnetic response. — For concreteness we study the effect of SO coupling on spin-triplet pairing originating from Hund's interaction, including the QP dispersion and the magnetic response. As discussed in the previous sections the qualitative results are generic for SO coupled t_{2g} -bands (or p -orbital systems) and can be applied to specific materials such as the single layer ruthenate [5, 6] and the Fe-pnictides [7, 30] using the appropriate band structure.

Using the kinetic Hamiltonian of eq. (10) with a parameter choice mimicking the single layer ruthenate band structure, the MF solutions for various λ are displayed in fig. 3. As one can see, in the absence of SO interaction an orbital-singlet spin-triplet pairing instability develops at a large coupling strength $3J - U \gtrsim 1.0$ for $\mathbf{d}_{xz/xy}$ and $\mathbf{d}_{yz/xy}$. Although numerically difficult to resolve, we expect that $\mathbf{d}_{yz/xz}$ and the intra-orbital spin-singlet order parameters simultaneously become finite through quartic or higher order couplings in the Landau free energy expansion. While the magnitudes of the order parameters depend on the details of the band structure, a robust fea-

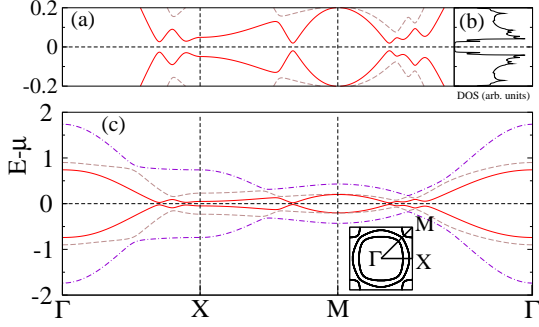


Fig. 4: (Color online) QP bands for $3J-U = 0.9$ and $\lambda = 0.15$. Panel (a) is a magnification of panel (c) about the Fermi level, revealing the gaps opening up on the FS sheets. Panel (b) shows the DOS and the QP gap near the Fermi level.

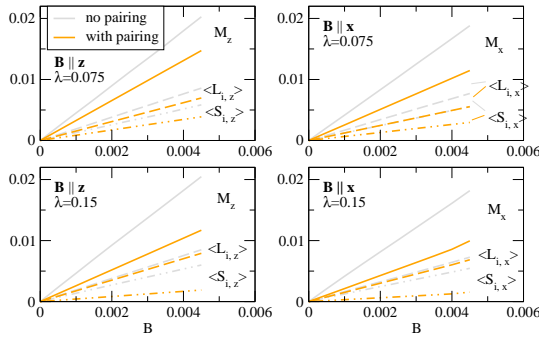


Fig. 5: (Color online) Magnetization parallel to the applied magnetic field \mathbf{B} for $\lambda = 0.075$ (top) and 0.15 (bottom) and two field orientations at $3J-U = 0.9$. The solid lines represent total magnetization, dashed lines stand for orbital contribution, and dash-dotted lines for spin magnetization. For sake of comparison the magnetic response both in the presence (orange) and in the absence (grey) of superconductivity is displayed. (B is expressed in units of $2t_1 = 1$.)

ture is that finite SO coupling drastically reduces the critical pairing strength. This reduction is mostly facilitated by the additional hybridization provided by H_{SO} , which helps to overcome the momentum mismatch between orbitals/bands near the Fermi level. On the other hand the same mechanism can have a slightly detrimental effect at larger $3J-U$, where the ideal inter-orbital pairing conditions along the diagonals are weakened by the additional hybridization. One may also wonder if the Bogoliubov QP dispersions have anisotropic gaps. The resulting QP bands are shown in fig. 4 and are fully gapped with a fourfold symmetric gap modulation in \mathbf{k} space, even though the gap minima are tiny.

Note that the present superconducting state does not break TRS. The magnetic response is a combination of paramagnetic (spin-triplet) and spin-singlet behaviours, with a slightly larger out-of-plane than in-plane total magnetic susceptibility as shown in fig. 5, where $\mathbf{M} = \langle \mathbf{L}_i \rangle + 2\langle \mathbf{S}_i \rangle$ is the total magnetization including orbital and spin contributions and $H_B = \mathbf{B} \cdot \sum_i (\mathbf{L}_i + 2\mathbf{S}_i)$ cou-

ples the orbital and spin degrees of freedom to the external field \mathbf{B} . Both orbital and spin expectation values are finite with roughly equal contribution to the total magnetization. For comparison, the normal state magnetizations are also shown in fig. 5 and are larger than in the superconducting state, as expected for a combination of spin-singlet and -triplet pairing in the presence of SO interaction. In particular, note that the spin magnetization changes drastically in the superconducting state with increasing λ . In general, the magnitude of the d -vectors, and thus the magnetic response, can be modified by changing the size of the FS sheets. For instance a larger overlap between yz and xy dominated portions of the FS would enhance $\mathbf{d}_{yz/xy}$ compared to $\mathbf{d}_{yz/xz}$ and $\mathbf{d}_{xz/xy}$. The spin susceptibility then would be mostly dominated by $\mathbf{d}_{yz/xy}$, a situation which may be facilitated by applying uniaxial pressure.

Discussion and summary. — Given that we based our MF study on the Sr_2RuO_4 compound to illustrate the effect of SO interaction on pairing, let us comment on the compatibility and the limitations of our results with what is known about the superconducting state in Sr_2RuO_4 [5, 6]. Based on the QP gap variation along the FS sheets, one expects that this modulation may also be reflected in orientation sensitive specific heat measurements. Such magnetic field dependent specific heat measurements on Sr_2RuO_4 have indeed been carried out [31, 32], but the interpretation of the experimental results is controversial, making a link to our QP dispersion difficult. However, due to the nature of inter-band pairing, the superconducting state presented here is sensitive to any kind of impurities associated with inter-band scattering, which is consistent with the phenomena observed in Sr_2RuO_4 .

Our result on the magnetization indicates that the spin-susceptibility is finite and different for in-plane and out-of-plane magnetic field orientations in both the normal and the superconducting state, as reported on Sr_2RuO_4 . Yet below T_c the in-plane and out-of plane susceptibilities decrease, which is in contrast to NMR Knight shift measurements [33, 34], which revealed that a change in the spin-response across T_c is absent for any field orientation. This behaviour differs also from the response expected of a chiral $p+ip$ superconductor, where the spin-susceptibility decreases for field directions perpendicular to the a - b plane but remains constant for parallel orientations. While the amount of change in the present model depends sensitively on the SO interaction strength, as shown in fig. 5, the question also arises as to how orbital and spin contributions were separated to obtain the Knight shift data when SO interaction is significant. Besides this, we note that the magnetic field effect on vortices will be highly non-trivial as well, as it involves competition between various types of vortices including half-quantum vortices [35, 36] in the presence of moderate SO coupling.

Finally, the lack of TRS breaking is compatible with the absence of chiral supercurrents as observed in scanning

Hall probe and scanning SQUID measurements [37, 38]. However, this contrasts with another proposal that the chiral states due to $p+ip$ pairing on α and β bands cancel each other leading to a topologically trivial superconductor [27]. It also contradicts Kerr rotation and μ SR measurements which have been interpreted in favour of TRS breaking [39, 40]. The issue as to whether TRS is broken or not is not yet resolved in the experimental community. While the current study supports a non-TRS breaking state, it can be modified by going beyond local interactions. A natural extension would be to include the effect of further neighbour ferromagnetic interactions such as those discussed by Ng and Sigrist [18], which could lead to a small admixture of odd parity pairing with broken TRS in addition to the pairing found here and which may be responsible for the broken TRS signatures found in μ SR and Kerr experiments [39, 40]. Another possibility is a finite-momentum pairing state such as a FFLO (Fulde-Ferrell-Larkin-Ovchinnikov) state [41, 42]. It is plausible that a FFLO state between different bands can be stabilized over the inter-band pseudospin-triplet pairing. These studies, and more definite predictions for Sr_2RuO_4 or other specific materials, however, go beyond the scope of the current 9 complex order parameter minimization and require more detailed work.

In summary, we studied the combined effect of Hund's and SO coupling on t_{2g} orbital systems. Three orbital-singlet spin-triplet pairings were found to form an orthogonal d -vector triad. A linear coupling between even-parity inter-orbital spin-triplet and even-parity intra-orbital spin-singlet pairings was allowed due to SO interaction, determining the orientation of the three d -vectors and giving rise to a relative phase difference of $\pi/2$ between spin-singlet and spin-triplet order parameters. We also showed that inter-orbital spin-triplet pairing in the orbital basis corresponds to even-parity inter- and intra-band pairing in the Bloch band basis, and discussed how the pairing strength varies within the Bloch bands. We further found that SO coupling assists Hund's coupling driven pairing, which generally leads to an anisotropic QP gap and an orbital dependent magnetic response.

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